CS 5220: Homework 2

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1 Initial Profiling

In order to perform initial profiling of the code before any improvements are made, Intel's VTUNE was used via the terminal command line on Totient. In an attempt to get the most accurate results (taken with a large sample size), we decided to gather data while running the large wave simulation, invoked with the command make big. Information collected from VTUNE's "advanced-hotspots" option is used in our analysis.

1.1 Whole Program - Advanced Hotspots

First, hotspots in the entire program were examined in order to determine where our efforts should be directed. The time taken in the top 10 most time consuming functions can be seen below in Figure 1. Of these, it is clear that most of our optimization efforts should be directed to the functions limited_derivs, compute_step, and compute_fg_speeds. These functions were then examined individually, once again using VTUNE on our advanced-hotspots collection.



Figure 1: Top 10 most time consuming functions in the wave simulation. Generated using Intel's VTUNE on Totient.

1.2 limited_derivs - Advanced Hotspots

The function limited_deriv is used to calculate the fluxes into and out of each cell in order to advance to the next time step. This involves a three point computational stencil in each direction and loops through the entire domain interior (the whole domain except for those where boundary conditions are applied). Each point requires $\mathtt{du.size}() \times 9$ floating point operations as well as $\mathtt{du.size}() \times 2$ calls to the intrinsic function min. Sadly, the hotspot

analysis on the limited_deriv function, shown in Figure 2, does not give any hints on possible optimizations or bottle necks.

Figure 2: Time taken to perform each loop present in limited_derivs, recorded in coreseconds.

1.3 compute_step - Advanced Hotspots

The purpose of compute_step is to update the wave equation to the next time step using a predictor-corrector method. First, the fluxes are calculated in the prediction. Next, the corrector step uses the predicted fluxes, the differences in velocities, and the current velocities, to advance to the next time state. Luckily, VTUNE's report is more helpful than in the previous case, and provides extensive timings for this function, shown in Figure 3. The calculation in the corrector step can be seen as the most expensive cost of the function. It is important to note, however, that the predictor step and copying of the solution to the u array sum to half of the function's cost.

1.4 compute_fg_speeds - Advanced Hotspots

The function of compute_fg_speeds has two primary responsibilities: to update the cell centered fluxes, f and g, and to calculate the maximum speed in the domain, allowing dynamic adjustment of the time step in order to satisfy the CFL condition and ensure numerical stability. The timing data for this function can be seen in Figure 4. While the most time consuming portion of the code is most likely the calculation of the fluxes and wave speed (both of which are in the Shallow2d structure), the calls to the intrinsic function max also represent a non-trivial amount of time.

Figure 3: Time taken to perform each loop present in compute_step, recorded in coreseconds.

Figure 4: Time taken to perform each loop present in compute_fg_speeds, recorded in core-seconds.

2 Parallelization

While we are aware that the optimal programming of this code will not wholly be due to parallelization by OpenMP, it is most certainly necessary. Furthermore, future tuning and optimization of the code may change depending on whether the code is run in serial or parallel. For these reasons, we first decided to parallelize the code and compare its performance against the initial, serial code.

2.1 Naive Implementation of OpenMP

First, a naive implementation of OpenMP using pragmas was used. This involved placing #pragma omp parallel for in front of the start of each for loop in the functions init, apply_periodic, compute_fg_speeds, limited_derivs, and compute_step. This proved to improve performance significantly when run on one node of Totient (24 threads), as seen in Figure 5. It should be noted that the time shown is the total processor time spent and not the per processor time.

Figure 5: Timing of entire simulation using naive implementation of OpenMP parallelized for-loops. Generated using Intel's VTUNE on Totient and recorded in core-seconds.

2.2 OpenMP for with collapse

"OpenMP parallel for" also has the collapse option, which essentially informs OpenMP how many nested loops are present. By knowing this, OpenMP is able to section both loops to run on multiple processors, creating blocks for each processor to work on. Results when using collapse can be seen in Figure 6. It should be noted that the time shown is the total processor time spent and not the per processor time. It was found that using the collapse option actually led to worse performance. We believe this is due to the creation of blocks, which will limit the amount of memory accesses each core has that is of unit stride. When only sectioning the for loops based on the vertical (y) direction, each processor gets a $n \times nx$ block of the array, where n is some number of rows (vertical lines of computational cells) in the domain. This increases memory access locality, which in turn increases cache hits.

2.3 OpenMP thread creation limited:

The constant creation of threads creates a large overhead cost that negatively affects the performance of the program. Therefore, the fewer times that a pool of threads needs to be created the better. In the previous examples, the thread pools were created each time a parallel for loop was called. In order to reduce this costly operation, a pool of threads was only created within the main run function as shown in the below code section.

```
        Central 20-Shallov20, Minifold (loat>>::compute_step
        shallow
        1346.237e

        _kmp_woil, templote-dwp_flog_64>
        libiomp5.so
        1265.233

        Central 20-Shallov20, Minifold (loat>>::limited_derivs
        shallow
        758.495

        Central 20-Shallov20, Minifold (loat>>:compute_fg_speeds
        shallow
        266.978

        Central 20-Shallov20, Minifold (loat>>::limidif
        shallow
        211.490s

        Cluttical only kinon module |
        [Unknown]
        173.865s
```

Figure 6: Timing of entire simulation using implementation of OpenMP parallelized forloops with collapse option. Generated using Intel's VTUNE on Totient and recorded in core-seconds.

```
for (int io = 0; io < 2; ++io) {
        real cx, cy;
        #pragma omp parallel
        apply_periodic();
        compute_fg_speeds(cx, cy);
        limited_derivs();
        #pragma omp single
            {
        if (io == 0) {
            dt = cfl / std::max(cx/dx, cy/dy);
            if (t + 2*dt >= tfinal) {
                dt = (tfinal - t)/2;
                done = true;
            }
        }
        compute_step(io, dt);
        #pragma omp single
        t += dt;
```

Sections of the code that only required one thread to execute took advantage of the omp single pragma command which tells only one thread to run that section of code while the rest wait for it to finish. Inside each of the computation calls the regular omp for pragma command is used to parallelize the various for loops being run. The performance of this operation for the top five costliest function calls when run on the big simulation can be found in Figure 7.

It should also be noted that these results do include the effects of attempting to force the compiler to vectorize several loops by replacing the min and max calls with an equivalent if statement min and max code. Also from Figure 7, it can be seen that the program still spends a large amount of time in block operations. Based on Figure 5, it appears that the main cost of thread creation is no longer one of the top performance issues with the code. Now, the internal barrier times is of much more concern.

Function	Module	CPU Time
[Events Lost On Trace Overflow]	Events Lost On Trace Overflow	176.770s
Central2D <shallow2d, minmod<float="">>::compute_step</shallow2d,>	shallow	100.152s
kmpc_barrier	libiomp5.so	98.943s
Central2D <shallow2d, minmod<float="">>::limited_derivs</shallow2d,>	shallow	76.487s
kmp_hyper_barrier_release	libiomp5.so	30.561s
[Unknown stack frame(s)]	[Unknown]	22.861s
Central2D <shallow2d, minmod<float="">>::compute fq speeds</shallow2d,>	shallow	20.214s

Figure 7: Timing of five costliest functions using fewer thread creation events. Generated using Intel's VTUNE on Totient.

2.4 OpenMP nowait implementation:

When using the omp_for pragma command, an implicit barrier is placed at the end of the loops. Due to the nature of this program, it is possible in several places to be able to assume that a barrier is not needed, and therefore the nowait pragma command can be used. The nowait command could be safely used in the compute_fg_speeds and limited_derivs functions. Then it could be partially used in the compute_step function once the predictor step was calculated. If the nowait command was used for the predictor loop, synchronization issues are possible when a thread is able to go onto the corrector step while other threads are still in the predictor step. The performance of this implementation for the top five costliest function calls when run on the "big" simulation can be found in Figure 8

Function	Module	CPU Time
[Events Lost On Trace Overflow]	Events Lost On Trace Overflow	173.308s
Central2D <shallow2d, minmod<float="">>::compute_step</shallow2d,>	shallow	109.107s
kmpc_barrier	libiomp5.so	73.633s
Central2D <shallow2d, minmod<float="">>::limited_derivs</shallow2d,>	shallow	63.533s
Central2D <shallow2d minmod<float="">>::compute for speeds</shallow2d>	shallow	40.003c

Figure 8: Timing of five costliest functions using nowait pragma command. Generated using Intel's VTUNE on Totient.

It can be seen by comparing Figure 7 and Figure 8 that the overall time spent in the barrier function call has gone down drastically by including the nowait call.

2.5 Thread Affinity:

OpenMP 4.0 offers the ability to describe the ordering of the threads among the CPUs/MICs. Threads can be placed near each other on the same CPU using the OpenMP pragma command procbind(close). The benefit of doing this is that amount of time for synchronization between threads should decrease. The downside of this is that the available cache and bandwidth per thread will decrease. Another option available distributes the threads more evenly throughout the available CPUs/MIC, and it can be turned on using the OpenMP pragma command procbind(spread). It should lead to the opposite effects of the close command. The thread affinity was implemented on the code base that used the nowait pragma command. The performance of this implementation for the top five costliest function calls when run on the big simulation can be found in Figure 9 and Figure 10 for the procbind(close) pragma command. Due to system traffic, timing can vary across multiple runs. For this reason, two figures were shown so some measure of variance could be judged. The results for the procbind(spread) command can be found in Figure 11.

Function	Module	CPU Time
[Events Lost On Trace Overflow]	Events Lost On Trace Overflow	166 0075
Central2D <shallow2d. minmod<float="">>::compute step</shallow2d.>	shallow	106.580s
kmpc_barrier	libiomp5.so	81.897s
Central2D <shallow2d, minmod<float="">>::limited_derivs</shallow2d,>	shallow	62.559s
Central2D <shallow2d, minmod<float="">>::compute fq speeds</shallow2d,>	shallow	39.688s

Figure 9: Timing of five costliest functions using proc_bind(close) pragma command for run 1. Generated using Intel's VTUNE on Totient.

Function	Module	CPU Time
[French Land On Town Owned] and	5t. 1t O. T Ofl	155 200-
[Events Lost On Trace Overflow]	Events Lost On Trace Overflow	
Central2D <shallow2d, minmod<float="">>::compute_step</shallow2d,>	shallow	112.596s
kmpc barrier	libiomp5.so	85.581s
Central2D <shallow2d, minmod<float="">>::limited_derivs</shallow2d,>	shallow	65.491s
Central2D <shallow2d. minmod<float="">>::compute fg speeds</shallow2d.>	shallow	43, 2975

Figure 10: Timing of five costliest functions using proc_bind(close) pragma command for run 2. Generated using Intel's VTUNE on Totient.

Overall, both thread affinity options have shown to lead to decreased performance. Therefore, they will not be used in the production code.

3 Analysis

The current implementation, while offering a sizable speed up over the strictly serial version, still leads much to be desired. Since it currently depends on the parallel for command to run with OpenMP automating certain commands, barriers are automatically placed into the code that limits how each processor accesses the memory of the variables. Further improvements can be made to the code by eliminating these blocking structures where allowed and only syncing the data when the need arises in order to reduce the amount of overhead costs that occur from this type of synchronization. One such place where this could be beneficial is in the compute_step function. Specific structures could be used in order to ensure the predictor step is done for edge cases before the corrector loop begins without requiring a barrier. To do this, a more rigorous implementation of OpenMP will need to be done, which mimics more of a distributed memory parallel code. Blocks will be made of the domain, where each subdomain has ghost cells and is unaware of what happens outside of itself (except through the ghost cells). This gives more control and limits necessary communication.

3.1 Strong and Weak Scaling

The current version of the code can be analyzed for its strong and weak scaling capabilities. The strong scaling will be tested using the "big" wave test case with 1000 points in each direction and 100 time steps between frames. The results can be seen in Table 1. This is tested on the main Xeon chips. With the highest number of threads tested being 16, internode communication costs were avoided. VTUNE analysis was also not collected in order to remove any additional time the collection process takes. In Table 1, strong scaling is defined by Eq. 1 and strong scaling efficiency is defined by Eq. 2.

Function	Module	CPU Time
[Events Lost On Trace Overflow]	Events Lost On Trace Overflow	119.259s
Central2D <shallow2d, minmod<float="">>::compute_step</shallow2d,>	shallow	104.188s
kmpc_barrier	libiomp5.so	100.178s
Central2D <shallow2d, minmod<float="">>::limited_derivs</shallow2d,>	shallow	62.695s
Central2D <shallow2d, minmod<float="">>::compute_fg_speeds</shallow2d,>	shallow	38.095s

Figure 11: Timing of five costliest functions using proc_bind (spread) pragma command. Generated using Intel's VTUNE on Totient.

Strong Scaling =
$$\frac{t_{\text{serial}}}{t_{\text{parallel}}}$$
 (1)

$$Strong Scaling = \frac{t_{\text{serial}}}{t_{\text{parallel}}}$$

$$Strong Scaling Efficiency = \frac{t_{\text{serial}}}{t_{\text{parallel}}} \frac{1}{p}$$

$$(2)$$

where t_{serial} and t_{parallel} are the times taken when running in serial or parallel, respectively, and p is the number of processors. The strong scaling efficiency is essentially what percentage of perfect linear scaling is actually achieved. This is plotted in Figure 12.

Threads	Total Time (seconds)	Strong Scaling	Strong Scaling Efficiency
1	539	1.0	100%
2	288	1.87	93.5%
4	218	2.47	61.7%
8	198	2.72	34.0%
16	188	2.87	17.9%

Table 1: Strong scaling for wave simulation with 1000 mesh points in each direction and 100 timesteps between frames.

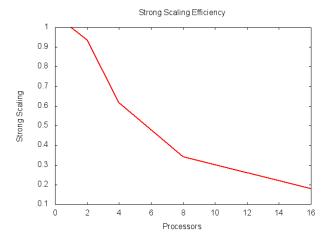


Figure 12: Plot of strong scaling, representing the data shown in Table 1.

For weak scaling, three simulations were performed, scaling the number of processors equally with the number of cells. The results can be seen in Table 2. Here, weak scaling is defined by Eq. 3. It was decided to double the side length for each simulation in order to perform the weak scaling test, meaning the number of processors needed to be quadrupled for each run. A plot of the weak scaling can also be seen in Figure 13. A more thorough weak scaling test is planned for the future.

Weak Scaling =
$$\frac{t_{\text{serial}}(n(p))}{t_{\text{parallel}}(n(p), p)}$$
(3)

Threads	Cells Per Side	Total Time (seconds)	Weak Scaling
1	200	4.0	1.00
4	400	8.3	0.485
16	800	73.5	0.0544

Table 2: Weak scaling for wave simulation with 1000 mesh points in each direction and 100 timesteps between frames.

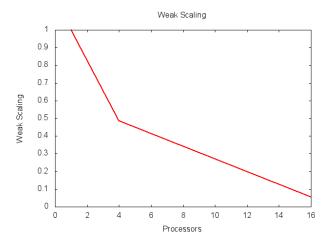


Figure 13: Plot of weak scaling, representing the data shown in Table 2.

We believe the weak scaling performance is very poor due to our implementation of OpenMP. Weak scaling usually tests the importance of communication on distributed memory systems, since each processor should be performing the same amount of algorithmic work as it is in the serial case. The main difference is the size of data being communicated is largely increased with the scaling in problem size. Since this is a shared memory code, we believe this indicates poor memory handling, leading to many cache misses. This is especially evident in the largest case, where we believe the problem size exceeded the cache size, causes very poor memory use. This could be fixed by a blocking scheme, where the domain is decomposed into subdomains, in order to increase memory locality, reducing the number of cache misses substantially. Another possible reason for the poor performance of

the 16 thread case is an increase in time for each communication, due to the threads existing on two separate chips.

The scaling can be represented theoretically by creating an equation for the parallel time taken in the code. This would be primarily made up of two parts: the time to perform the floating point operations, and the portion spent communicating and synchronizing. In this code, since it uses shared memory, the only communications required involves OpenMP barriers and informing each processor of their section of the "for loops". These communications will be incorporated into the relation using the variable t_c . Predicting the value of t_c consistently is difficult due to uncertainty in how long processors will be required to wait at a barrier. Through running simulations with various parameters, it may be possible to get a rough estimate of the communication time per processor, which could then be used in this model to approximate the scaling for a specific simulation.

The expression for time taken to execute the simulation in parallel can be represented by Eq. 4.

$$t_{\text{parallel}} = \frac{t_{\text{serial}}}{p} + pt_c \tag{4}$$

This equation assumes that the serial work will be evenly distributed among all processors, leading to the serial work being completed in $t_{\rm serial}/p$ time. The cost of parallelizing the code per processor, in the form of communication, barriers, and synchronization, is represented by t_c . With an expression for the parallel time, it is now possible to create a rough approximation for scaling, shown in Eq. 5. The difference in strong and weak scaling appears in the values used for $t_{\rm serial}$ and t_c .

Scaling
$$\approx \frac{t_{\text{serial}}}{t_{\text{parallel}}} = \frac{t_{\text{serial}}}{\frac{t_{\text{serial}}}{p} + pt_c} = \left(\frac{1}{p} + p\frac{t_c}{t_{\text{serial}}}\right)^{-1}$$
 (5)

4 Post Initial Report Work:

4.1 Swapping Programming Languages:

Due to the problems that the layer of abstraction within C++ code base gave the compiler, it was decided it would be best to transition over to Professor Bindel's C version of the code. The initial results from that swap resulted in a set of code that was performing at the same level of performance as the parallelized C++ code when using 16+ threads. Therefore, this code base will provide an appropriate environment to see what effects various forms of parallelization can have on the performance on the code.

4.2 Vectorization and other optimizations of the code base:

While the C code is rather vectorized, it still had a couple of areas of improvement that could be made to allow the compiler to better vectorize the various loops in the code. First off, the various techniques used in the matmul assignment can be introduced here including aligning the memory to a 32 byte boundary and the use of the # pragma vector aligned command. The _mm_malloc() and _mm_free() commands were used in place

of the malloc and free commands for the creation of the sim and sim->u variables. This allowed the compiler to know that these variables would be aligned to a 32 byte boundary. Also since several other variables are based upon the sim->u, the compiler recognizes that these also should be aligned to a 32 byte boundary as well. Next, the # pragma vector aligned is used at each for loop used in both the stepper.c and shallow2d.c files. Since all the vector variables with initial data have been aligned, the various calculations done inside the loop will not lead to a segmentation fault. If this was not the case, the __attribute__((aligned(32))) would want to be used during the declaration of those variables in order to ensure those variables were aligned. It should also be noted that if the Xeon Phi chips were being used than the vectors could be aligned to a 64 byte boundary instead, since the chip set supports the AVX512 instruction set. Finally, the following Intel compiler optimization flags were used to ensure we are taking full advantage of the Xeon architecture during our vectorization attempts:-O3 -axcore-avx2-march=core-avx2 -unroll-aggressive -m64 -ipo -no-prec-div -ansi-alias.

Next, several times a variable is created inside a for loop. This constant creation of these variables could lead to a slow down of the code. Therefore, if the variable being created did not call for the use of the const or restrict keywords it was initially created outside of the loop(s). This move was done for both the stepper.c and shallow2d.c file. The results when comparing the baseline C code, and the further optimized code can be seen in Table 3 for a 1000x1000 size mesh. It can be seen while the speed up is minor it is a nice improvement on an already well optimized code base.

Simulation Name	Time(s)	Speed up(%)
Baseline Code	59.8	100
Aligned Code	55.9	107

Table 3: Comparison of baseline and aligned C code bases for a simulation with a 1000 mesh points and 50 frames

4.3 Naive OpenMP Implementation:

A naive OpenMP implementation was used initially in this code base where no subdomain blocking has yet to be implemented. The purpose of this is to see what effects parallelization techniques will have on an already fairly well optimized code base with good performance. The OpenMP implementation will be based upon the best implementation used in the C++ code base. Although, one of the major differences will be that the user can now directly specify the number of threads to use when the program runs. The main shallow2d run function now looks like the following:

```
#pragma omp single
central2d_periodic(u, nx, ny, ng, nfield);
speed(cxy, u, nx_all * ny_all, nx_all * ny_all);
dt = cfl / fmaxf(cxy[0]/dx, cxy[1]/dy);
if (t + 2*dt >= tfinal) {
    dt = (tfinal - t)/2;
    done = true;
}
}
central2d_step(u, v, scratch, f, g,
               0, nx+4, ny+4, nq-2,
               nfield, flux, speed,
               dt, dx, dy);
central2d_step(v, u, scratch, f, q,
               1, nx, ny, ng,
               nfield, flux, speed,
               dt, dx, dy);
#pragma omp single
t += 2*dt;
nstep += 2;
}
```

It was then found that the following functions could contain a parallelized for loop: central2d_step, central2d_correct_sd, limited_deriv1, and limited_derivk. The various other functions contained in here if parallelized would lead to negative height being seen. Also, it should be noted that loop counter variable needed to be declared outside the loop and then declared private for the C code. The actual results of implementing this will be seen in the weak and strong scaling subsection, but it should be noted that this implementation resulted in a vastly slower performance. It needs to also be noted that when the mesh becomes more refined an increase in threads will lead to a height less than 0 assertion to happen. This was discovered when trying to run the weak scale study. One explanation could be that a nonintuitive race condition is occurring that is allowing the one thread change the value of variable that another thread has yet gotten to use yet. However, the OpenMP implementation of a barrier at the end of each for loop should prevent this from occurring.

4.4 Weak and Strong Scaling for C code:

The strong scaling for the naive OpenMP implementation can be seen in Table 4 and Figure 14. It can be seen that the parallelization has led to a degradation in performance and this can be mainly contributed to the communication cost between threads. Also, it is not as

large of a factor anymore the constant creation of threads is also a problem. One thing that should also be noted is that since a less than 0 assertion can be reached for larger mesh sizes the strong scaling done for the C code base is not 1:1 to the one done for the C++ code base.

Threads	Total Time (seconds)	Strong Scaling	Strong Scaling Efficiency(%)
1	2.39	1.00	100.0
2	11.40	0.21	10.0
4	20.71	0.12	3.0
8	25.03	0.10	1.0
16	31.13	0.08	0.5

Table 4: Strong scaling for wave simulation with 400 mesh points in each direction and 50 timesteps between frames.

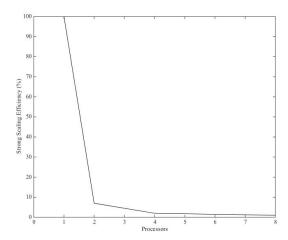


Figure 14: Plot of weak scaling, representing the data shown in Table 4.

Next, the weak scaling can be seen in Table 5 and Figure 15. A couple more points were obtained for this study by taking a $\sqrt{2}$ increase in cell size in order to be able to just double the number of threads. It can also be seen from this table that the naive implementation of OpenMP had detrimental effects on the performance of the code.

It can be seen from these scalings that in order to even attempt at getting better performance out of the code a subdomain implementation of OpenMP will need to be used.

5 Future Work

Once the code has been parallelized with subdomains using OpenMP, use of the Xeon Phi chips will be implemented in the code. Thus far, we have had trouble using the Xeon Phi

Threads	Cells Per Side	Total Time (seconds)	Weak Scaling(%)
1	200	0.35	100
2	283	5.11	7
4	400	17.70	2
8	566	55.61	1

Table 5: Weak scaling for wave simulation with 50 frames and N varying mesh size.

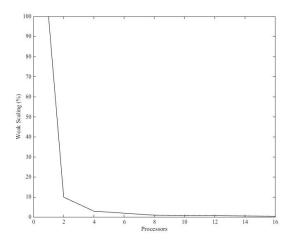


Figure 15: Plot of weak scaling, representing the data shown in Table 5.

chips via the #pragma offload target (mic:0) command. We are not entirely sure of the issue, but believe it has to do with the use of templates in the C++ version of the code.

Once the code is parallelized into subdomains and effectively offloaded to the Xeon Phi chip, we will attempt to vectorize the loops. Preliminarily, we have had trouble vectorizing the loops within the C++ memory structure currently used, and have not managed to use the restrict keyword. Without this, the compiler is easily confused about dependencies inside the loop, as it cannot be sure where separate pointers are pointing to. It may be necessary to switch to the C version of the code that was written by Professor Bindel in order to tune the code for better vectorization.